Computational electrocatalysis: methods and fundamental applications on CO2 reduction and formic acid oxidation
Granda Marulanda, L.P.

Citation

Version: Publisher's Version
License: Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden
Downloaded from: https://hdl.handle.net/1887/3217519

Note: To cite this publication please use the final published version (if applicable).
LIST OF PUBLICATIONS, CONFERENCES AND AWARDS

Publications

Chapter 2

Chapter 3

Chapter 4

Chapter 5

Chapter 6

Conferences

69th Annual Meeting of the International Society of Electrochemistry
Electrochemistry from Knowledge to Innovation, 2 to 7 September 2018. Bologna, Italy
Laura Granda Marulanda, Xiaoting Chen, Ian McCrum, Federico Calle-Vallejo, Marc Koper. Insights into HCOOH Oxidation and HCOOH Production from CO2 on PdML/Pt-based Electrocatalysts from Theoretical and Experimental Studies. [poster]

Awards

HPC-Europa3 Transnational Access programme -2019
A scholarship to promote collaborations within the theoretical/computational scientific community within Europe. Awarded with computing time in the MareNostrum super computer in Barcelona. Hosted by Dr. Federico Calle-Vallejo of the Institute of Theoretical and Computational Chemistry of the Universitat de Barcelona (IQTCUB)

ISE poster prize -2018
Poster prize at the 69th Annual Meeting of the International Society of Electrochemistry in Bologna, Italy.
Academiegebouw van de Universiteit Leiden
The Netherlands
ACKNOWLEDGEMENTS

I remember very well the sunny day in September 2016 when I came to Leiden for my interview. I had missed the bus stop to the university and ended up a few blocks away. I was panicking because I got lost, but I finally made it to the interview. Finishing my PhD is just the beginning of a new chapter, but it is also the closure of a 12-year chapter of my life. It started when I enrolled the graduate program at Texas A&M back in 2009, then I took a longer path, but that allowed me to see the other side of the world (literally), a world I never imagined I will live in. This opportunity made me grew on a personal and professional level and allowed me to finish my graduate studies.

In that respect I would like to thank first my supervisor, Marc Koper for giving me the opportunity to pursue the doctorate degree in the CASC group, and most importantly for your personal and professional support, for your understanding, for being open and available for discussions and for the freedom to do research. Also, thank you for encouraging me to attend the summer school in Denmark, one of the most enriching experiences during my PhD. Thank you for bringing up the questions- the puzzles, which helped me tremendously to stay focused and on the right track within my noisy mind.

I am honored to have pursued graduate studies and research at Leiden University and for the emerged collaborations, friendship and support from all past and present colleagues. Isis, the first person I met from the CASC group, thank you for agreeing to meet me before all this started, for answering all my questions related to life in Leiden and for encouraging me to pursue my PhD journey. Federico Calle-Vallejo, thank you for your guidance during the first year of my journey, where I was very lost in space and time, ☝️, thank you for helping me prioritize my goals. But mostly I am enormously grateful for encouraging me to apply to the HPC3 program, and for the fruitful collaboration it led to. There I got momentum, and confidence to continue this journey and I strongly believed that without that opportunity I would not be where I am now. From you I’ve learned that DFT and modelling in electrocatalysis is very complex, but still, it can be simple and fun. I learned the importance of testing and how to discern data. Thank you for all the time helping me improving and correcting my manuscripts and chapters of my thesis and for the very insightful “consejos de vida” (life tips). Ian McCrum, thanks for sharing your contagious passion and excitement for science, for the many fun discussions and for supporting my dreams of opening a company, and even if it does not materialize, I am grateful for the inspirational chats we had regarding to that. For your availability to discuss science, for teaching me computational electrocatalysis, DFT and the analysis of experimental data from a practical lens. For helping me improve my presentations and manuscripts and for your cheerful famous quotes; “you can do whatever you want” and “I have faith in you”. Xiaoting Chen, thank you for all your hard work and research that led to beautiful science and collaboration, thank you for your patience in waiting for my DFT results ☺️, and for our chats and discussions over lunch. Selwyn, thank you for teaching me the statistical thermodynamics needed for my scripts, and for helping me during the first months of my PhD to set up my computer and have it ready to go. Thank you for the work discussions and for being always available to help. Miss. José, thank you a lot for all the personal and technical support you offered me, I am so grateful for your help in finding a temporal place to stay in Leiden and for sharing your knowledge and passion about plants. A very huge thanks to my A-leaf friends from the CASC group, Thomas and Amanda for sharing special moments in our A-leaf meetings and for making those enjoyable, thanks for your support and friendship.

To all my previous mentors: Nelson Granda, José Cortés-Figueroa, Phill Bhüllman, Manuel Soriaga, James Bateas, and Igor Paští. I am deeply grateful for the learning and research opportunities I had with you, for your mentorship and guidance before I started the PhD. Those opportunities were turning points that led me to this stage.
To all the CASC past and present members, postdocs, fellows, students and technical staff that I have met since my start: Adrien, Akansha, Alisson, Amanda, Arthur, Asad, Cásia, Charlotte, Christoph, Chunming, Dajo, Damien, Davide, Diana, Diyu, Elena, Eli, Federico, Francesc, Giulia, Ian, Jan, Jess, José, Kasmith, Katharina, Koen, Leon, Mahesh, Sabine W., Marcel, Mariana, Marta, Mathias, Matthijs, Mehdi, Nakkiran, Rafael, Richard, Sabine A., Setwyn, Sileia, Stefan, Steven, Thom, Thomas, Vlad, Wentian, Xiaoting, Xin, Yohan, Yuvaraj and Zhiqin. Thank you all for all the work discussion, chats over lunch, cake breaks, coffee breaks, beers at the science club or the mathematics building, for the Potluck dinners, for the group outings and for priceless experiences like the summer and winter schools and conferences we attended together. Thank you for making the CASC group a very pleasant working environment and for making my PhD more enjoyable in the Netherlands.

Special thanks to my colleagues and friends Diana, Jess, Stefan, Giulia, Matías, Amanda, and Ian. Thank you for all the shared moments and memories we built together also outside the working hours. Some of you from the start and some of you at the end of my journey. Thank you for your generous friendship. For those long walks in the city center and around the lakes of Leiden, for the sushi dinners and the movie nights. I learned from you about life and research. Diana and Jess, first thanks for the analytical chemistry conversations, and python code fixes, but most importantly thank you for being there during my darkest and happiest moments during this journey and for the constant encouragement to keep moving forward and not give up.

To my friends outside university: Monique and Lilián, my soul sisters, thank you for spicing up my life in The Netherlands, for understanding me and for being there in the good and bad. You have taught me to balance PhD life with life. I am grateful for all the laughs and tears we shared, the wines and tequilas and deep conversations about life.

To all my caring and supportive friends: Alexis, Melissa, Tatiana, Linda, Kethura, Mavreen, Milagros, Heçgli, Leslie, Andrea, Natalia, Nancy, Lina, Marianne, Ceci, Leda, Desi, Kristhell, Saraht, and Dorde, thank you for teaching me so many things about life and myself, I would need a new chapter to write all our memories but I want to let you know that I am thankful for the support provided at all different stages of this journey.

To my beloved partner in crime: Ivica Milovanović, out of the 12 years of this journey, we did 11. Thank you for all your support, love and care- even on your hardest and difficult moments. Thank you for encouraging me to pursue computational chemistry, for all the chemistry discussions and for teaching me some fancy functional programming for my scripts. Thank you for always pushing me to keep becoming a better person, to “follow my heart”, and most importantly, for overcoming many obstacles together, and accompanying me in The Netherlands.

A mi querida familia, mis padres y mis hermanos a los que adoro mucho. Mami y papi, gracias por darme todas las herramientas necesarias para poder construir mis alas y volar. A pesar de todo el esfuerzo que requiere emigrar de Colombia y hacer la maestría en un nuevo país y además con dos hijos, nunca me faltó su apoyo y cariño. Gracias por enseñarme a ser persistente y precavida y sobre todo por apoyarme a lograr y perseguir mis metas. Les dedico esta tesis con todo mi corazón, mis logros son sus logros.

A my soul sisters, thank you for all the laughs and tears we shared, the wines and tequilas and deep conversations about life.

To all my caring and supportive friends: Alexis, Melissa, Tatiana, Linda, Kethura, Mavreen, Milagros, Heçgli, Leslie, Andrea, Natalia, Nancy, Lina, Marianne, Ceci, Leda, Desi, Kristhell, Saraht, and Dorde, thank you for teaching me so many things about life and myself, I would need a new chapter to write all our memories but I want to let you know that I am thankful for the support provided at all different stages of this journey.

To my beloved partner in crime: Ivica Milovanović, out of the 12 years of this journey, we did 11. Thank you for all your support, love and care- even on your hardest and difficult moments. Thank you for encouraging me to pursue computational chemistry, for all the chemistry discussions and for teaching me some fancy functional programming for my scripts. Thank you for always pushing me to keep becoming a better person, to “follow my heart”, and most importantly, for overcoming many obstacles together, and accompanying me in The Netherlands.

A mi querida familia, mis padres y mis hermanos a los que adoro mucho. Mami y papi, gracias por darme todas las herramientas necesarias para poder construir mis alas y volar. A pesar de todo el esfuerzo que requiere emigrar de Colombia y hacer la maestría en un nuevo país y además con dos hijos, nunca me faltó su apoyo y cariño. Gracias por enseñarme a ser persistente y precavida y sobre todo por apoyarme a lograr y perseguir mis metas. Les dedico esta tesis con todo mi corazón, mis logros son sus logros.

To all my caring and supportive friends: Alexis, Melissa, Tatiana, Linda, Kethura, Mavreen, Milagros, Heçgli, Leslie, Andrea, Natalia, Nancy, Lina, Marianne, Ceci, Leda, Desi, Kristhell, Saraht, and Dorde, thank you for teaching me so many things about life and myself, I would need a new chapter to write all our memories but I want to let you know that I am thankful for the support provided at all different stages of this journey.

To my beloved partner in crime: Ivica Milovanović, out of the 12 years of this journey, we did 11. Thank you for all your support, love and care- even on your hardest and difficult moments. Thank you for encouraging me to pursue computational chemistry, for all the chemistry discussions and for teaching me some fancy functional programming for my scripts. Thank you for always pushing me to keep becoming a better person, to “follow my heart”, and most importantly, for overcoming many obstacles together, and accompanying me in The Netherlands.

A mi querida familia, mis padres y mis hermanos a los que adoro mucho. Mami y papi, gracias por darme todas las herramientas necesarias para poder construir mis alas y volar. A pesar de todo el esfuerzo que requiere emigrar de Colombia y hacer la maestría en un nuevo país y además con dos hijos, nunca me faltó su apoyo y cariño. Gracias por enseñarme a ser persistente y precavida y sobre todo por apoyarme a lograr y perseguir mis metas. Les dedico esta tesis con todo mi corazón, mis logros son sus logros.

To all my caring and supportive friends: Alexis, Melissa, Tatiana, Linda, Kethura, Mavreen, Milagros, Heçgli, Leslie, Andrea, Natalia, Nancy, Lina, Marianne, Ceci, Leda, Desi, Kristhell, Saraht, and Dorde, thank you for teaching me so many things about life and myself, I would need a new chapter to write all our memories but I want to let you know that I am thankful for the support provided at all different stages of this journey.

To my beloved partner in crime: Ivica Milovanović, out of the 12 years of this journey, we did 11. Thank you for all your support, love and care- even on your hardest and difficult moments. Thank you for encouraging me to pursue computational chemistry, for all the chemistry discussions and for teaching me some fancy functional programming for my scripts. Thank you for always pushing me to keep becoming a better person, to “follow my heart”, and most importantly, for overcoming many obstacles together, and accompanying me in The Netherlands.
Laura Patricia Granda Marulanda was born on 9th June 1988 in Cali, Colombia. At the age of 6 she moved to Puerto Rico where she completed her high school and bachelor education. She enrolled the Chemistry program from the university of Puerto Rico at Mayagüez graduating in 2009. During this period, she did an internship at the university of Minnesota in the USA under the LANDO program and worked on the project “Design of a solid-contact ion selective electrode for the detection of perfluoroalkyl acids”. From 2009 to 2011 she enrolled graduate studies and worked as a teacher assistant in the Chemistry department at Texas A&M. There, her preliminary research involved fundamental studies of silicate minerals using the Atomic Force Microscope. Later, fascinated by the world of computational chemistry, she redirected her research interests and enrolled the faculty of Physical Chemistry at the University of Belgrade in Serbia, where she completed her master’s degree in 2013 on the project: “Theoretical study of the interaction of PtTM dimers (TM = Ru, Rh, Pd, Ir and Pt) with MgO(001) surface - adsorption, mobility and electronic structure”.

In January 2017, Laura started her PhD in the CASC group, Leiden University, The Netherlands under the supervision of prof. dr. M. T. M. Koper. The main results obtained during this graduate research are described in this thesis, presented at international conferences and published in scientific journals.

Besides science, Laura enjoys long walks, dancing salsa and bachata, doing Zumba®, pole fitness, and loves to gaze at the horizon. She used to play the oboe, and now she is learning the ukulele. She also enjoys listening to informative podcasts and reading.